

# Integral Transforms from Finite Data: An Application of Gaussian Process Regression to Fourier Analysis

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## Abstract

Computing an accurate estimate of the Fourier transform of a continuum-time signal from a discrete set of data points is crucially important in many areas of science and engineering. The conventional approach of performing the discrete Fourier transform of the data has the shortcoming of assuming periodicity and discreteness of the signal. In this paper, we show that it is possible to use Gaussian process regression for estimating any arbitrary integral transform without making these assumptions. This is possible because the posterior expectation of Gaussian process regression maps a finite set of samples to a function defined on the whole real line. In order to accurately extrapolate, we need to learn the covariance function from the data using an appropriately designed hierarchical Bayesian model. Our simulations show that the new method, when applied to the Fourier transform, leads to sharper and more precise estimation of the spectral density of deterministic and stochastic signals.

## 1. Introduction

While measurements are always discrete and finite in number, data analysts, physicists and engineers often model signals as being defined on the whole time axis. In fact, the sampling frequency and the range of the samples only pertains to the measurement process and not to the signal itself. The Fourier transform is perhaps the most important methodological tool for the analysis of signals. To estimate the Fourier transform of the underlying continuous-time signal, one often uses the discrete Fourier transform (DFT). However, the DFT only provides an unbiased estimate if that underlying continuous-time signal is periodic and contains no frequencies above the Nyquist frequency (Rabiner and Gold, 1975). In this paper, we introduce a Bayesian method for estimating the continuum-time Fourier transform (or any other continuum-time linear transform) of continuum-time and discretely sampled signals based on Gaussian processes (GP) regression (Rasmussen, 2006). The estimation procedure assumes neither periodicity nor discreteness of the latent signal and outputs a function expressed as a linear combination of tractable kernel functions. This latter feature is particularly important since it allows to perform a wide range of further analysis analytically using closed-form expressions, thereby reducing the impact of numerical errors and instabilities on the analysis pipeline.

## 1.1 Related works

Bayesian methods have become very influential in the field of spectral estimation (Gregory and Mohammad-Djafari, 2001). Recently some work has been done on the use of GP regression for stochastic spectral estimation of continuum-time signals. These methods are based on a parametric (Wilson and Adams, 2013) or non-parametric (Tobar et al., 2015) estimation of the covariance function, since the spectral density of a stochastic process can be directly obtained from its covariance function (Rasmussen, 2006). The aim of this class of methods is to estimate the spectral density of a stochastic process. As such, they cannot be used for estimating the Fourier transform. Our approach can be seen as a generalization of the GP quadrature method, that uses GP regression for numerical integration of definite integrals (O’Hagan, 1991). In this approach, the function to integrate is assumed to be sampled from a GP distribution and evaluated on a finite set of points. Importantly, under these assumptions, the posterior distribution of the integral can be obtained in closed-form.

## 2. Background

The Fourier transform of a continuum-time (real or complex valued) function  $f(t)$  is defined as follows:

$$\mathfrak{F}[f(t)](\omega) = f(\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-i\omega t} f(t) dt , \quad (1)$$

where  $e^{-i\omega t} = \cos \omega t - i \sin \omega t$  is a complex valued sinusoid. The Fourier transform is a linear operator. We can interpret the Fourier transform as a special case of (linear) integral transform. A more general integral transform can be defined as follows:

$$\mathfrak{I}_{\mathcal{A}}[f(t)](s) = \int_b^a \mathcal{A}(s, t) f(t) dt , \quad (2)$$

where the bivariate function  $\mathcal{A}(s, t)$  is the kernel of the transform. The limits of integration,  $a$  and  $b$ , can be finite or infinite.

### 2.1 Gaussian Process Regression

GP methods are popular Bayesian nonparametric techniques for regression and classification. A general regression problem can be stated as follows:

$$y_t = f(t) + \epsilon_t , \quad (3)$$

where the data point  $y_t$  is generated by the latent function  $f(t)$  plus a zero-mean noise term  $\epsilon_t$  that we will assume to be Gaussian. The main idea of GP regression is to use an infinite-dimensional Gaussian prior (a GP) over the space of functions  $f(t)$ . This infinite-dimensional prior is fully specified by a mean function, usually assumed to be identically equal to zero, and a covariance function  $\mathfrak{K}(t, t')$  that specifies the prior covariance between two different time points. The posterior distribution over  $f(t)$  can be obtained by applying Bayes theorem. Given a set of training points  $(t_k, y_k)$ , it can be proven that the posterior expectation  $m_f(t)$  is a finite linear combination of covariance functions:

$$m_f(t) = \sum_k w_k \mathfrak{K}(t, t_k) , \quad (4)$$

where the weights are linear combinations of data points

$$w_k = \sum_j A_{kj} y_j . \quad (5)$$

In this expression, the matrix  $A$  is given by the following matrix formula:

$$A = (K + Q)^{-1} , \quad (6)$$

where  $Q$  is the covariance matrix of the noise and the matrix  $K$  is obtained by evaluating the covariance function for each couple of time points

$$K_{ij} = \mathfrak{K}(t_j, t_k) . \quad (7)$$

The derivation of these results is given in (Rasmussen, 2006).

### 3. Computing Integral Transforms Using GP Regression

One of the most appealing features of GP regression is that, while the training data are finite and discretely sampled, the posterior expectation is defined over the whole time axis. Furthermore, Eq. 4 shows that this expectation is a linear combination of covariance functions. From this linearity, it follows that every integral transform of  $m_f(t)$  can be calculated as a linear combination of the integral transform of the covariance functions  $\mathfrak{K}(t, t_k)$ :

$$\begin{aligned} \mathcal{I}_{\mathcal{A}}[m_f](s) &= \int_b^a \mathcal{A}(s, t) \left[ \sum_k w_k \mathfrak{K}(t, t_k) \right] dt \\ &= \sum_k w_k \int_b^a \mathcal{A}(s, t) \mathfrak{K}(t, t_k) dt . \end{aligned} \quad (8)$$

Clearly, this transform is well-defined as far as the transform  $\int_b^a \mathcal{A}(s, t) \mathfrak{K}(t, t_k) dt$  exists. To the best of our knowledge, we are the first to suggest the use of GP regression for computing an arbitrary integral transform. However, the special case where the integral operator is a simple definite integral has been applied to numerical integral analysis and it is known as the GP quadrature rule (O'Hagan, 1991):

$$\int_b^a f(t) dt \approx \sum_k w_k \int_b^a \mathfrak{K}(t, t_k) dt . \quad (9)$$

The form of the GP covariance function can be learned from the data in order to obtain better extrapolation and interpolation performance. For example, learning the frequency and waveform of a quasi-periodic signal allows to extrapolate beyond the training time points, thereby increasing the spectral resolution. Therefore we will outline a hierarchical Bayesian method for estimating the covariance function directly from the measurements.

### 3.1 Hierarchical Covariance Learning

The aim of this subsection is to introduce a hierarchical Bayesian model that allows to estimate the GP covariance function from the data. We restrict our attention to stationary covariance functions, i.e. covariance functions that solely depend on the difference between the time points  $\tau = t' - t$ . We construct the hierarchical model by defining a hyper-prior distribution over the spectral density  $\mathfrak{S}(\xi)$ , defined as the Fourier transform of the covariance function:

$$\mathfrak{S}(\xi) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathfrak{K}(\tau) e^{-i\xi\tau} d\tau . \quad (10)$$

Since the Fourier transform is invertible, an estimate of the spectral density can be directly converted into an estimate of the covariance function. Using a GP hyper-prior on the spectral density  $\mathfrak{S}(\xi)$  would be a convenient modeling choice as it easily allows to specify the prior smoothness, thereby regularizing the estimation. For example, we could use a GP hyper-prior with squared exponential (SE) kernel (covariance) function:

$$\mathfrak{K}_{SE}(\xi, \xi') = e^{-\frac{(\xi - \xi')^2}{2\sigma^2}} , \quad (11)$$

where the scale parameter  $\sigma$  regulates the prior smoothness. Unfortunately, this GP prior is not proper since it assigns non-zero probability to negative valued spectra, which do not correspond to any valid stationary stochastic process. However, we can obtain a proper prior distribution by restricting this GP probability measure to the following positive-valued functional sub-space:

$$\{\mathfrak{s}(\xi) = \sum_j e^{a_j} \mathfrak{K}_{SE}(\xi, \xi_j) | a_j \in \mathbb{R}\} , \quad (12)$$

where  $\xi_j$  are the discrete Fourier frequencies of the sampled data points. Using the resulting prior distribution, we calculate the maximum-a-posteriori (MAP) estimate by means of a gradient ascent algorithm applied to the posterior distribution of the spectral density given the sampled data points. This iterative algorithm maximizes the posterior distribution with respect to the (log)weights  $a_j$  and therefore only finds a solution in the restricted subspace in Eq. 12. Note that, for calculating the MAP estimate, we do not need to know the density of the restricted prior distribution; it is sufficient to know a function that is proportional to it, as in our case. The resulting MAP estimate has the following form:

$$\hat{\mathfrak{S}}(\xi) = \sum_j e^{h_j} \mathfrak{K}_{SE}(\xi, \xi_j) , \quad (13)$$

where  $h_j$  are the optimized log-weights. Finally, our point estimate of the covariance function is obtained by applying the inverse Fourier transform to the MAP estimate:

$$\begin{aligned} \hat{\mathfrak{K}}(\tau) &= \int_{-\infty}^{+\infty} e^{i\xi\tau} \hat{\mathfrak{S}}(\xi) d\xi \\ &= \sum_j e^{h_j} \int_{-\infty}^{+\infty} e^{i\xi\tau} \mathfrak{K}_{SE}(\xi, \xi_j) d\xi \\ &= \sigma \sum_j e^{h_j} e^{-\frac{\sigma^2\tau^2}{2} - i\xi_j\tau} . \end{aligned} \quad (14)$$

This covariance function has the advantage of capturing the spectral features of the data while keeping a tractable analytic expression as a linear combination of the inverse Fourier transforms of SE kernel functions. Note that, if we have access to multiple realizations of a stochastic time series, we can learn the spectral density from the whole set of realizations simply by summing the log marginal likelihood of each realization. We will use this procedure in our analysis of neural oscillations.

### 3.2 Bayes-Gauss-Fourier transform

We can now plug-in the data-driven covariance function in our expression for the integral transform and exploit the linear structure of the covariance function by interchanging summation and integration:

$$\mathfrak{I}_{\mathcal{A}}[m_f](s) = \sigma \sum_{k,j} w_k e^{h_j} \int_b^a \mathcal{A}(s, t) e^{-\frac{\sigma^2(t-t_k)^2}{2} - i\xi_j(t-t_k)} dt. \quad (15)$$

In the case of the Fourier transform, this formula specializes to

$$\mathfrak{F}[m_f](\omega) = \sigma^2 \sum_{k,j} w_k e^{h_j} e^{-\frac{(\omega-\xi_j)^2}{2\sigma^2} - i\omega t_k}, \quad (16)$$

because

$$\mathfrak{F}\left[e^{-\frac{\sigma^2(t-t_k)^2}{2} - i\xi_j(t-t_k)}\right](\omega) = e^{-\frac{(\omega-\xi_j)^2}{2\sigma^2} - i\omega t_k}.$$

We refer to the resulting transformation of the data as the Bayes-Gauss-Fourier (BGF) transform.

## 4. Experiments

In this section we validate our new method on simulated and real data. We focus our validation studies on the problem of estimating the power spectrum of deterministic and stochastic signals, as this is perhaps the most common application of the Fourier transform.

### 4.1 Analysis of a noise-free signal

We investigate the performance of our method in recovering the Fourier transform of a discretely sampled deterministic signal. As our example signal, we use the following an-harmonic windowed oscillation  $g(t) = e^{-\frac{t^2}{2a^2}} \cos^3 \omega_0 t$ . We sampled the signal from  $t_{min} = -25$  to  $t_{max} = 25$  in steps of 0.01 and with  $a = 15$  and  $\omega_0 = \frac{3}{5}\pi$ . These samples were analyzed using the BGF transform as described in the Methods. Fig. 1A shows the result of the GP regression in the time domain. Clearly, the expected value of the GP regression (blue line) is able to extrapolate the waveform of the signal far beyond the data points. Next, we compared our GP-based estimate with two more conventional estimates of the spectrum  $|g(\omega)|^2$ : the Discrete Fourier Transform (DFT) of the data using a square and a Hann taper. Fig. 1B shows these spectral estimates, together with the ground truth spectrum, on a log scale. The BGF transform (green line) captures the shape and width of the four main lobes almost perfectly, despite the fact that their peaks are not fully

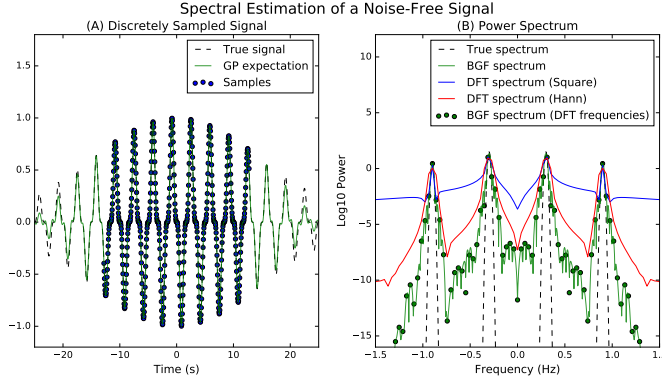


Figure 1: Spectral estimation of a synthetic signal. A) Ground truth signal (dashed black line), sample points (blue dots) and the expected value of the GP regression (green line). B) (Log10) Power spectrum of the ground truth signal (dashed line) and spectral estimates obtained from the samples using BGF transform (green line), DTF with square taper (blue line) and DTF with Hann taper (red line).

aligned with the discrete Fourier frequencies of the sampled data (which are determined by the signal’s length). Furthermore, the BGF transform has significantly higher sidelobe suppression than the DFT estimates, up to  $10^6$  higher than the DFT with Hann taper.

## 4.2 Analysis of a noisy signal

We evaluated the robustness of the method to noise in the time series. As our ground truth signal, we used again the deterministic signal given in the previous subsection, but we corrupted the observation with Gaussian white noise ( $\text{sd} = 0.1$ ). We compare the performance of the BGF transform with the performance of a popular multitaper estimator involving discrete prolate spheroidal sequences (DPSS) (Percival and Walden, 1993). We included the DPSS multitaper estimation for this analysis of noisy signals because that method is able to increase the reliability of the noisy estimates by means of spectral smoothing. Fig. 2A shows that the GP expected value acts as a denoiser and remains able to extrapolate the signal beyond the data points. As the noisy data require more regularization, the amplitude of the oscillation is reduced. Fig. 2B shows the estimated spectrum. The recovery of the main lobes remains very accurate, except for a small downward shift due to the amplitude loss. Furthermore, the flat background noise spectrum is more suppressed as compared to the multitaper estimates.

## 4.3 Fourier analysis of neural oscillations

In this section, we show that the BGF transform leads to sharper and less noisy estimates of the spectrum of neural oscillations. We collected resting state MEG brain activity from an experimental participant that was instructed to fixate on a cross at the center of a black screen. The study was conducted in accordance with the Declaration of Helsinki and

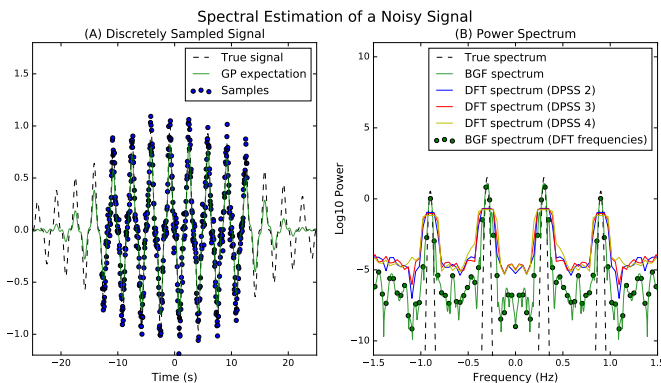


Figure 2: Spectral estimation of a synthetic noisy signal. A) Ground truth signal (dashed black line), noise-corrupted sample points (blue dots) and expected value of the GP regression (green line). B) (Log10) Power spectrum of the ground truth signal (dashed line) and spectral estimates obtained using BGF transform (green line), DTF with square taper (blue line) and DTF with two (blue line), three (red line) or four (yellow line) DPSS tapers

approved by the local ethics committee (CMO Regio Arnhem-Nijmegen). Since we are not interested in the spatial aspects of the signal, we restricted our attention to the analysis of the MEG sensor with the greatest alpha (10 Hz) power. We analyzed the time series using the BGF transform. In this analysis, the covariance function of the GP was estimated jointly from all trials by summing the trial specific likelihoods. We compared the resulting spectral estimates with those obtained by using DPSS multitaper DFT (with 3 tapers). Fig. 3 shows the average and standard deviation of the log power estimates. From the figure we can see that, compared to the DPSS multitaper estimate (panel B), the spectral peaks of the BGF estimate (panel A) are sharper and more clearly visible against the  $1/f$  background.

## 5. Discussion

In this paper we introduced a new method for performing integral transforms of a continuum-time signal that we have observed in a finite number of samples. While the method can be applied to any linear transform, we mostly focused our exposition on the Fourier transform, which is of great applied and theoretical importance. One of the most important features of our approach is that the output of the BFG transform is a continuous function that can be further analyzed using analytic methods.

Having at our disposal a continuous instead of a discrete function is particularly valuable because the Fourier transform is often an intermediate step in a more complex analysis. One interesting example is signal deconvolution, which can be performed exactly if we can obtain the analytic expression of the inverse Fourier transform of the ratio between the kernel function and the convolution filter in the frequency domain.

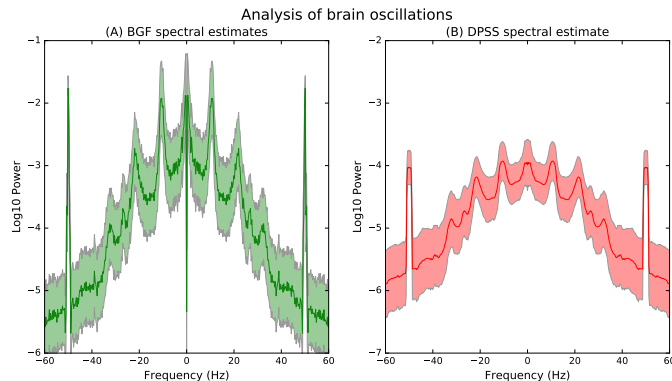


Figure 3: Analysis of human MEG signal. 1) (Log) Spectral estimate obtained using BGF transform. 2) (Log) Spectral estimate obtained using DPSS DTS with three tapers.

The performance of our method in recovering accurate spectral estimates greatly relies on the fact that we determine the covariance function of the GP using the MAP estimate of a hierarchical Bayesian posterior. In this way, we automatically detect the presence of quasi-periodicity in the signal and we use this information to extrapolate the signal outside of the range of the measurements.

The good performance of the BGF transform encourages the application of the method to other integral transforms such as the Laplace, the continuum-time wavelet and the Hilbert transform (Daubechies, 1990; Davies, 2002; Boashash, 1992). The estimation of all these integral transforms from finite data is an ill-posed problem and can be regularized by our Bayesian approach. In the case of the Hilbert transform, the present work connects with one of our previous works where we introduced a probabilistic reformulation of this integral transform based on GP regression (Ambrogioni and Maris, 2016).

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